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A QUANTITATIVE METHOD FOR CALIBRATING CFD MODEL CALCULATIONS

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Abstract

Computational fluid dynamics (CFD) modeling is being used more frequently in fire protection engineering design. The increase of CFD usage in fire protection engineering can be attributed in part to advances in computer hardware as well as the use of computationally efficient approaches for modeling fire phenomena such as the large eddy simulation technique utilized in NIST's Fire Dynamics Simulator (FDS). An important consideration in the use of CFD modeling is the calibration of model results. Calibration typically involves comparisons made between model calculations and experimental data sets. These comparisons are often characterized qualitatively using terms such as "good agreement" or "reasonable agreement." Such qualitative results provide little guidance in applying the calibration results to other situations. Therefore, a quantitative method for model calibration could provide better guidance to CFD modelers on the appropriate use of stated results.

Two quantitative approaches to CFD model calibration using linear regression and relative error are presented. The two methods are demonstrated by using FDS version 3 (FDS3) to model scenarios similar to McCaffrey's fire plume correlation and Alpert's ceiling jet correlation. The calculated temperature and velocity values from FDS were compared to the results of the correlations. The quality of each comparison was quantified using linear regression analysis to compute the square of the Pearson product moment correlation coefficient, commonly referred to as R^2, and the mean relative error. The influence of computational grid cell size, or mesh density, on the results calculated by FDS has also been examined. The methods presented in this work can be used by CFD modelers to quantify the results of calibration studies as well as to provide guidance on selecting an appropriate grid cell size when temperature and velocity are the variables of interest.

Keywords: Calibration, Ceiling jets, Computational fluid dynamics, Fire dynamics simulator, FDS, Fire plumes, Fire Modeling

1. Introduction

The process of calibrating CFD model results typically involves comparing calculated results to known values from experimental data, empirical results or analytical expressions. The McCaffrey fire plume (Drysdale, 1996) and the Alpert ceiling jet (Evans, 1995) correlations were modeled with NIST's Fire Dynamics Simulator version 3 (McGrattan *et. al.*, 2002). The use of a method common in linear regression analysis as well as a method of mean relative error will be investigated for their suitability in quantifying the degree of agreement between calculated and known values.

In linear regression analysis the quality of a curve fit to a given data set is usually referred to in terms of the square of the Pearson product moment correlation coefficient, or R^2 (Holman, 1994). The Pearson product moment correlation coefficient is

$$R = \frac{n\left(\sum XY\right) - \left(\sum X\right)\left(\sum Y\right)}{\sqrt{\left[n\sum X^2 - \left(\sum X\right)^2\right]\left[n\sum Y^2 - \left(\sum Y\right)^2\right]}} \qquad \text{Eq. 1}$$

Where R is the Pearson product moment correlation coefficient, n is the number of data points, X is the value of a known data point, and Y is a calculated value. The closer the value of R^2 is to unity, the better the correlation is between the known and calculated values. In the ideal situation where the calculated values are exactly the same as the known values at each point (i.e., X=Y), the value of R^2 would be 1. It should be noted that the computation of R^2 is typically a native function in spreadsheet programs and therefore, can be easily implemented when analyzing data.

In addition to the R^2 method the calculated data sets will also be analyzed using the mean relative error. The error for an individual point is computed in the following manner:

$$E = \frac{(Y - X)}{X}$$

Eq. 2

Where E is the relative error and X and Y are the known and calculated values, respectively. The mean relative error, E_m is computed using the absolute values of the error in the individual points. Therefore, in situations where an over-prediction and an under-prediction are of the same magnitude, the net result in the error will not be zero.

$$E_m = \frac{\sum\left(\left|\frac{Y - X}{X}\right|\right)}{n}$$

Eq. 3

The quantitative methods for comparing calculated results to known values described above can be applied to model verification as well as grid sensitivity studies. Grid sensitivity is an important issue in determining the optimal grid spacing for a particular problem. A grid spacing that provides a grid-independent solution in a CFD calculation represents a balance between minimizing numerical error and minimizing CPU time expenditure. One extreme example would be a very coarse grid spacing (i.e., few grid cells) leading to calculations with large numerical error due to insufficient resolution of physical phenomena being completed in a relatively short period of time. An example of the other extreme would be a very fine grid spacing (i.e., many grid cells) leading to calculations with minimal numerical error because the relevant length scales have been resolved and a large CPU time to complete the simulation. The use of a quantitative method in a grid sensitivity study could help identify an appropriate grid spacing using a metric of further grid refinement producing only marginal improvements in predicted quantities while increasing the computational expense. The examples that follow demonstrate the use of the suggested quantitative methods but do not fully investigate model verification or grid sensitivity.

2. Example: McCaffrey Plume Correlation

McCaffrey's fire plume correlation is based on experiments conducted with a 0.3m square methane diffusion burner with heat release rate values in the range of 14.4 to 57.5kW (Drysdale, 1996). Therefore, the bounding heat release rate values of 14.4 and 57.5kW were modeled with FDS3. The physical domain was 0.6m by 0.6m in plan and the height was twice the distance to the intermittent/plume interface according to regions defined in McCaffrey's correlation. The height of the domain for the 14.4 and 57.5kW scenarios was 1.20 and 1.95, respectively. The computational domain was based on uniform grid spacing in all three coordinate directions in multiples of 0.15m. For each heat release rate value six different grid spacings were evaluated with FDS3. The six grid spacings (dx) were 15, 10, 7.5, 5, 3, and 1.5cm for all three coordinate directions of each cell. This range represents a span of one order of magnitude in terms of grid cell dimensions.

A total of 15 measurement locations were used for both centerline temperature and velocity in the plume. In each region of the fire plume – flame, intermittent, and plume – five equidistant measurement points were used. The same 15 measurement point locations were used to compute the centerline temperature and velocity with McCaffrey's correlation in order to make a comparison between the correlation and the FDS3 calculation.

The graphical results for the FDS3 calculation relative to the correlation for centerline temperature and velocity are shown in Fig. 1 and 2 for the 14.4kW case and in Fig. 3 and 4 for the 57.5kW case. The results of the R^2 and mean relative error analysis are summarized in Tables 1 and 2 for the 14.4 and

57.5kW cases, respectively. The most favorable results, defined as R^2 closest to 1 and E_m closest to 0, appear in bold text.

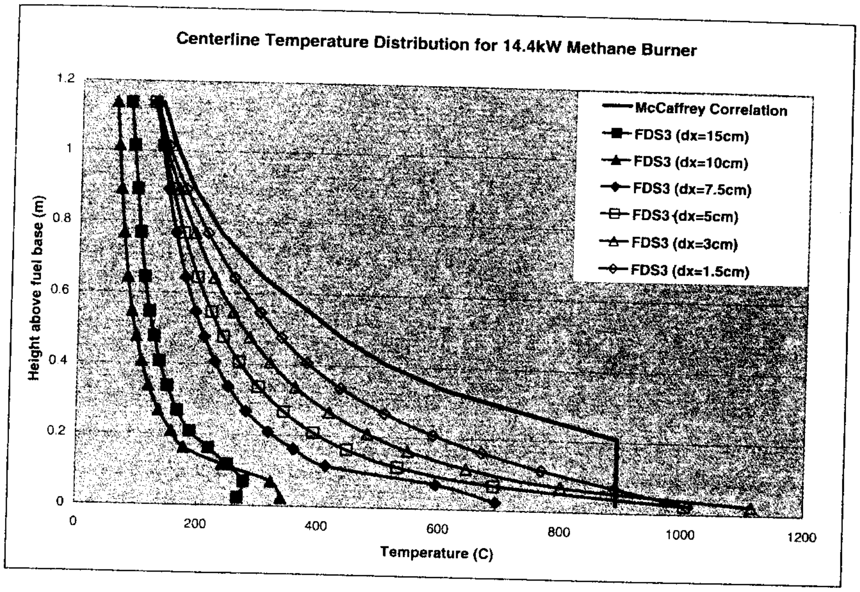

Fig.1 Centerline temperature distribution for McCaffrey correlation and FDS3 calculations with 14.4kW fire.

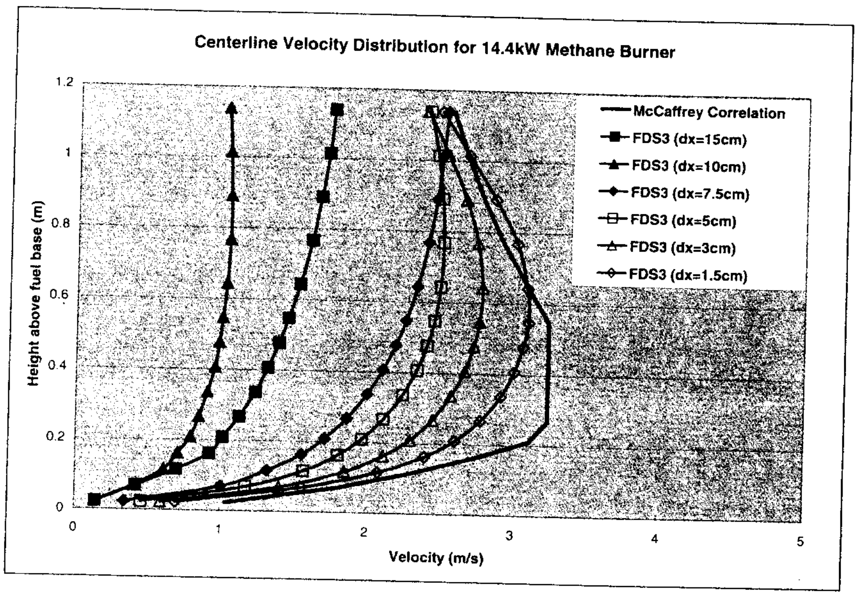

Fig.2 Centerline velocity distribution for McCaffrey correlation and FDS3 calculations with 14.4kW fire.

Table 2. R^2 and mean relative error in temperature and velocity calculations for 14.4kW fire at each grid spacing.

dx (cm)	R^2 (temp)	R^2 (vel)	E_m (temp)	E_m (vel)
15	0.863	0.500	0.660	0.579
10	0.690	0.709	0.723	0.705
7.5	0.679	0.593	0.424	0.322
5	0.646	0.753	0.354	0.264
3	0.716	0.871	0.281	0.173
1.5	**0.865**	**0.923**	**0.179**	**0.091**

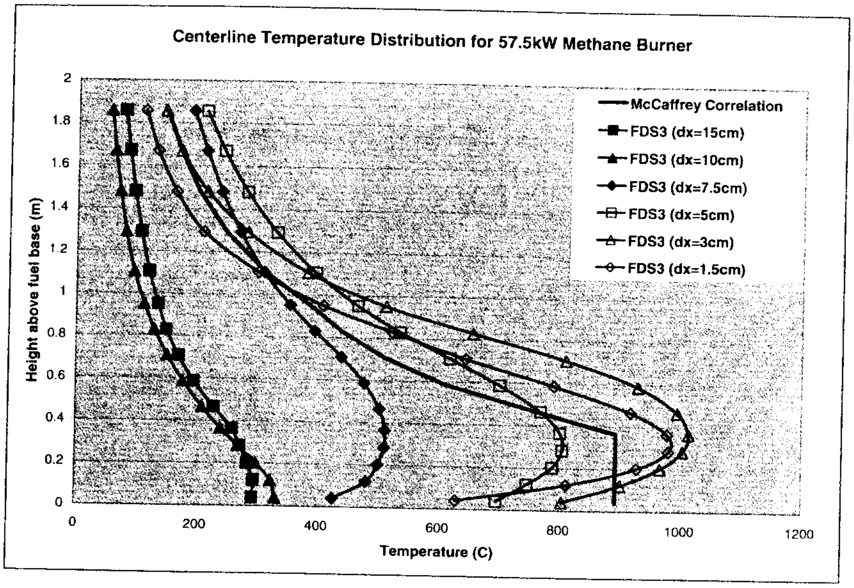

Fig.3 Centerline temperature distribution for McCaffrey correlation and FDS3 calculations w ith 57.5kW fire.

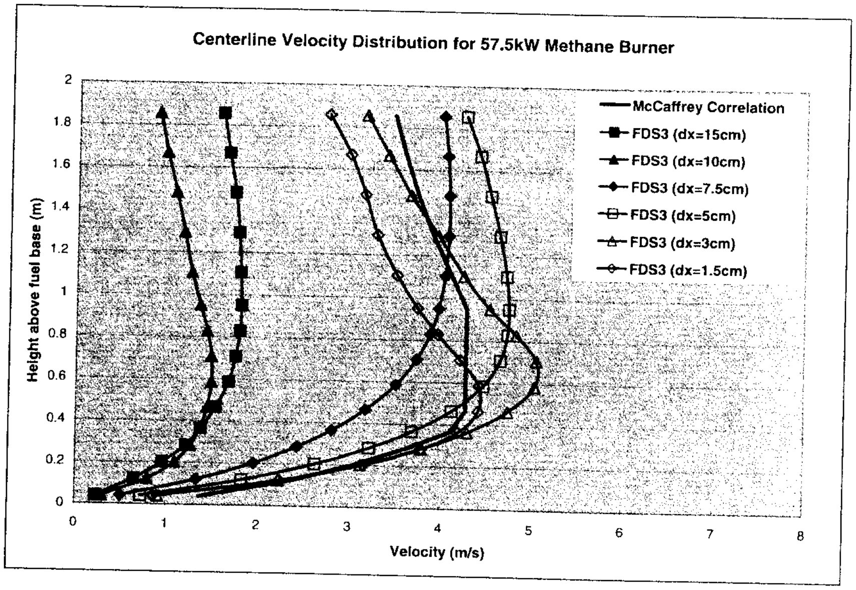

Fig.4 Centerline velocity distribution for McCaffrey correlation and FDS3 calculations with 57.5kW fire.

Table 2. R^2 and mean relative error in temperature and velocity calculations for 57.5kW fire at each grid spacing.

Dx (cm)	R^2 (temp)	R^2 (vel)	E_m (temp)	E_m (vel)
15	**0.986**	0.851	0.632	0.620
10	0.940	0.885	0.680	0.686
7.5	0.863	0.692	0.268	0.216
5	0.932	0.854	0.225	0.163
3	0.875	**0.953**	0.211	**0.092**
1.5	0.884	0.870	**0.165**	0.110

From Fig. 1 and 2 it can be seen that qualitatively the FDS3 calculations with 1.5cm grid spacing shows the best agreement with the correlation for centerline temperature and velocity. Additionally, the results in Table 1 show that there is agreement between the most favorable R^2 and mean relative error as well as with the qualitative assessment of Fig. 1 and 2. From Fig. 3 and 4 it is difficult to discern whether the 5, 3, or 1.5cm grid spacing has the best agreement with the correlation. There is agreement between the most favorable R^2 and E_m values in Table 2 for the centerline velocity and this result is reasonable given the qualitative assessment. However, there is disagreement between the most favorable values of R^2 and E_m results for the centerline temperature. The most favorable result of E_m for centerline temperature at 1.5cm grid spacing agrees with the qualitative assessment unlike the most favorable R^2 value at 15cm.

3. Example: Alpert Ceiling Jet Correlation

Two scenarios similar to the experiments that form the basis of Alpert's ceiling jet correlation were modeled with FDS3 and compared to the correlation with the same methods used for McCaffrey's plume correlation. The first scenario was a 1m by 1m 670kW ethanol fire under a 7m high unconfined ceiling. The planar dimensions of the domain were 14m by 14m with the fire located in the center of the domain. This allowed for a range of ceiling jet values up to an r/H of 1. Four uniform grid spacings (dx) of 50, 33.3, 25 and 20cm were used in the FDS3 modeling.

The graphical results of the correlation relative to the FDS3 calculations for maximum ceiling jet temperature and velocity are shown in Fig. 5 and 6. The r/H values correspond to 7 radial locations from 1 to 7m in 1m increments. The results of the R^2 and mean relative error analysis are summarized in Table 3 with the most favorable result appearing in bold text.

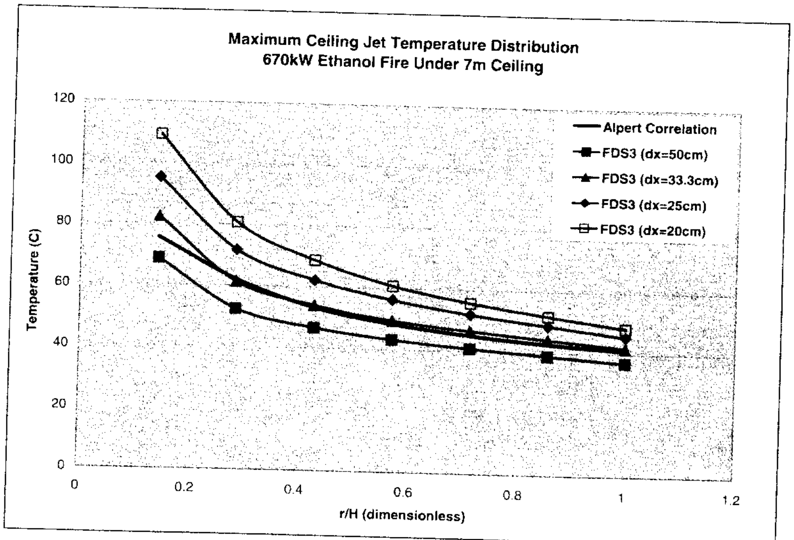

Fig.5 Maximum ceiling jet temperature distribution for Alpert correlation and FDS3 calculations with 670kW fire.

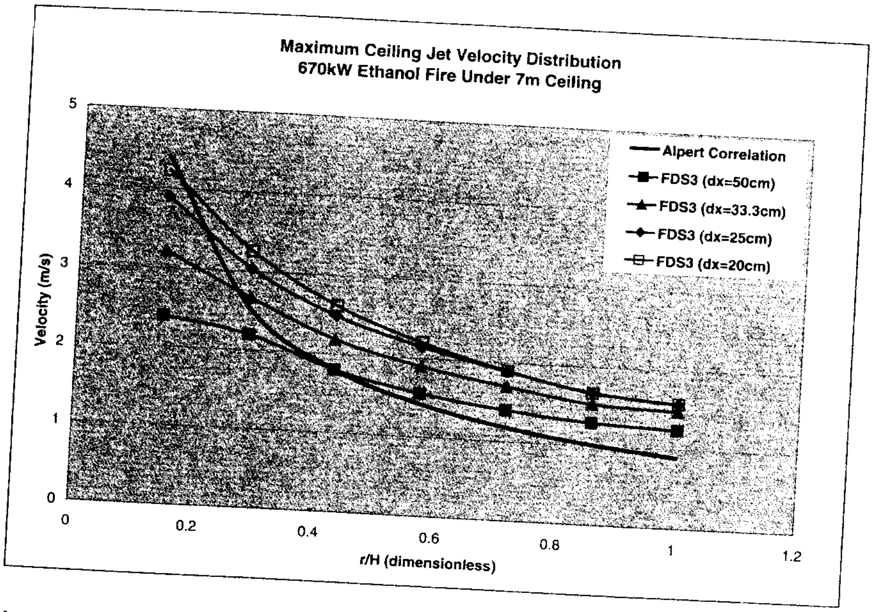

Fig.6 Maximum ceiling jet velocity distribution for Alpert correlation and FDS3 calculations with 670kW fire.

Table 3. R^2 and mean relative error in temperature and velocity calculations for 670kW fire at each grid spacing.

dx (cm)	R^2 (temp)	R^2 (vel)	E_m (temp)	E_m (vel)
50	0.983	0.879	0.108	**0.218**
33.3	0.981	0.948	**0.033**	0.353
25	0.992	**0.966**	0.163	0.458
20	**0.994**	0.965	0.274	0.477

Fig. 5 shows that the 33.3cm grid spacing has the best agreement with the correlation for maximum ceiling jet temperature. Fig. 6 shows that the 50cm grid spacing has the best agreement with the correlation for maximum ceiling jet velocity. However, there is no consistent agreement between R^2 and E_m for either temperature or velocity in Table 3. The most favorable results of E_m for both temperature and velocity are consistent with the qualitative assessment. The most favorable values of R^2 are not consistent with the qualitative assessment.

The second scenario was a 0.6m by 0.6m 1,000kW heptane fire under a 7.2m high unconfined ceiling. The planar dimensions of the domain were 14.4m by 14.4m with the fire located in the center of the domain. As in the first scenario this allowed for a range of ceiling jet values up to an r/H of 1. Three uniform grid spacings of 60, 30, and 20cm were used in the FDS3 modeling.

The graphical results of the correlation relative to the FDS3 calculations for maximum ceiling jet temperature and velocity are shown in Figures 7 and 8. The r/H values correspond to 12 radial locations from 0.6 to 7.2m in 0.6m increments. The results of the R^2 and mean relative error analysis are summarized in Table 4 with the most favorable result appearing in bold text.

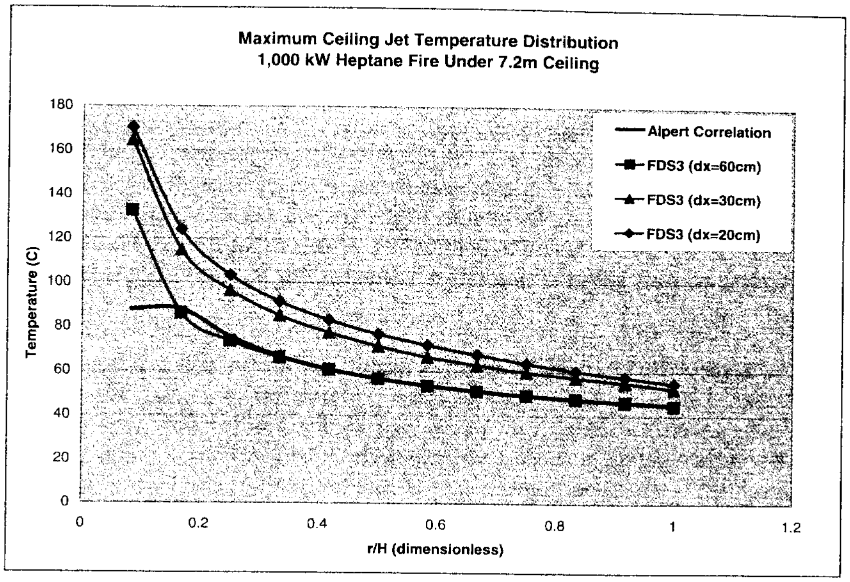

Fig.7 Maximum ceiling jet temperature distribution for Alpert correlation and FDS3 calculations with 1,000kW fire.

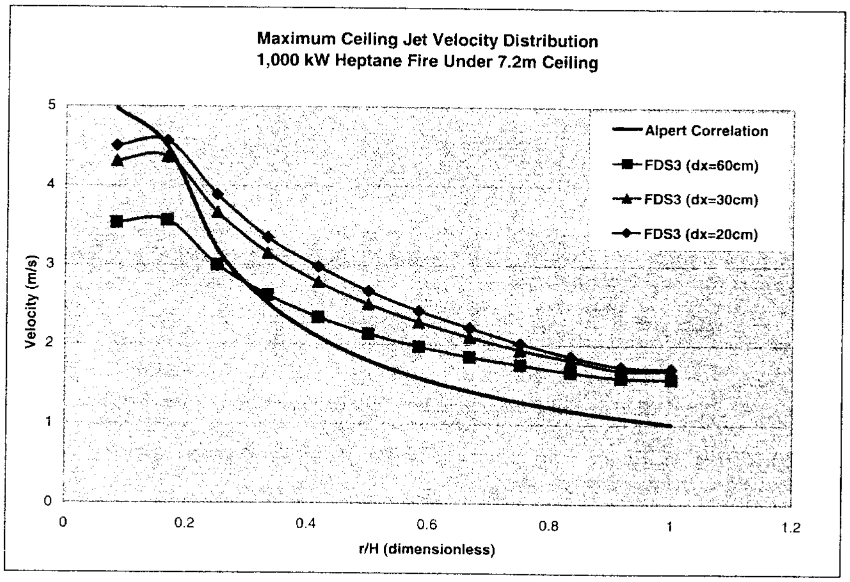

Fig.8 Maximum ceiling jet velocity distribution for Alpert correlation and FDS3 calculations with 1,000kW fire.

Table 4. R^2 and mean relative error in temperature and velocity calculations for 1,000kW fire at each grid spacing.

dx (cm)	R^2 (temp)	R^2 (vel)	E_m (temp)	E_m (vel)
60	0.798	**0.973**	**0.049**	**0.272**
30	0.864	0.963	0.292	0.373
20	**0.891**	0.951	0.375	0.425

Fig.7 and 8 show that the 60cm grid spacing exhibits the best agreement with the correlation for both maximum ceiling jet temperature and velocity on a qualitative basis. The most favorable values of R^2 and E_m for maximum ceiling jet velocity in Table 4 are consistent with one another as well as with the qualitative assessment. However, for maximum ceiling jet temperature in Table 4 the most favorable values of R^2 and E_m are not consistent with one another. The most favorable value of E_m is consistent with the qualitative assessment.

Conclusions

In all four cases analyzed the mean relative error method exhibited the best agreement with the qualitative assessment for both temperature and velocity. This was shown for both near field phenomena in the McCaffrey plume as well as for far field phenomena in the Alpert ceiling jet. Although the concept of using R^2 as a quantitative measure to compare CFD calculated values to a known data set appears to be a logical, the results of the analysis do not support this method. It was shown in both the 57.5kW plume case and in both ceiling jet cases that the most favorable R^2 value for temperature was not consistent with the qualitative assessment of the calculated values relative to the correlation.

The mean relative error method could be used in model verification and grid sensitivity studies to quantify the comparison between CFD calculations and a known set of values. For model verification work the mean relative error method provides a numerical value for how well a CFD calculation compares to a known data set for a specific variable such as temperature or velocity. As seen in the two examples presented in this paper, proper care should be given to specify the regions where such comparisons were made, i.e., fire plume, ceiling jet, etc. In terms of grid sensitivity studies the mean relative error method can be used to select which grid spacing is appropriate for a particular scenario. The improved accuracy of finer grid spacing can be weighed against the increased computational time and help provide a quantitative basis for making decisions on appropriate grid cell size.

It should be noted that the fire plume and ceiling jet examples were presented for the sole purpose of demonstrating the suitability of the R^2 and mean relative error analysis techniques. The examples should not be considered to be comprehensive model verification studies nor should the most favorable result from any example be considered as the optimal grid spacing for a particular problem.

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